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Notes

Computing Sadhana polynomial of V-phenylenic nanotubes and nanotori

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The Sadhana polynomial is defined as $Sd(G,x) = \sum_c m(G,c) \cdot x^{|E|-c}$, where m(G, c) is the number of strips of length *c*. This new polynomial has been defined to evaluate the Sadhana index of a molecular graph. The relation between this new polynomial and Omega polynomial is investigated. In particular, a method of computing Sadhana polynomial and then Sadhana index for V-phenylenic nanotubes and nanotori with given parameters m and n has been described.

The unique properties of carbon nanotubes have made this new form of solid carbon the most studied nano-material for the past few years.[1,2] They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted tremendous academic and industrial interest. It is, thus, of interest to study the mathematical properties of these materials.

In recent years, several papers have been published on the mathematical properties of nanotubes. Some authors computed the Wiener, Szeged, Balaban, Schultz and PI indices of nanotubes and nanotori while others have studied their kekulé structures.[3-13] Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures.[14-16] This theory had an important effect on the development of the chemical sciences. In the present Note, an attempt has been made for studying nanostructures by using graph theory.

Methodology

In this section, we recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. Suppose G is a connected molecular graph and x, y ∈ V(G). The distance *d*(x,y) between x and y is defined as the length of a minimum path between x and y. Two edges e = ab and f = xy of G are called codistant, "e co f", if and only if *d*(a,x) = *d*(b,y) = k and d(a,y) = *d*(b,x) = k+1 or vice versa, for a non-negative integer k. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive.

Set C(e):= {f ∈ E(G) | f co e}. If the relation "co" is transitive on C(e) then C(e) is called an orthogonal cut "oc" of the graph G. The graph G is called co-graph if and only if the edge set E(G) is the union of disjoint orthogonal cuts. The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by Diudea as Ω (G, x) = Σ_cm(G, c) × x^c, with m(G,c) being the number of strips of length *c*. The summation runs up to the maximum length of qoc strips in G. If G is bipartite, then a qoc starts and ends out of G and so Ω(G, 1) = *r* /2, in which *r* is the number of edges in out of G (refs 17-20).

The Sadhana index Sd(G) for counting qoc strips in G was defined by Khadikar *et al.*[21,22] as Sd(G)= Σ_c m(G,c)(|E(G)|−*c*), where m(G,c) is the number of strips of length *c*. We now define the Sadhana polynomial of a graph G as Sd(G,x)=Σ_c m(G,c) $x^{|E|-c}$) By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$ in Omega polynomial. Then the Sadhana index will be the first derivative of Sd(G, x) evaluated at x = 1.

The aim of this study is to compute the Sadhana polynomial and then Sadhana index of V-phenylenic nanotubes and nanotori. To do this, we first draw these compounds by HeperChem[23] and then compute their adjacency and distance matrices by TopoCluj[24]. Next, we apply some GAP[25,26] programs to compute the number of parallel edges for a given edge of these nanomaterials. Final step of this process is analyzing data obtained by our GAP programs. These programs are accessible from the authors upon request.

Herein, our notation is standard and taken from the standard book of graph theory and related studies[27-31].

Results and discussion

The Sadhana polynomial of a V-phenylenic nanotube and nanotorus were computed as described

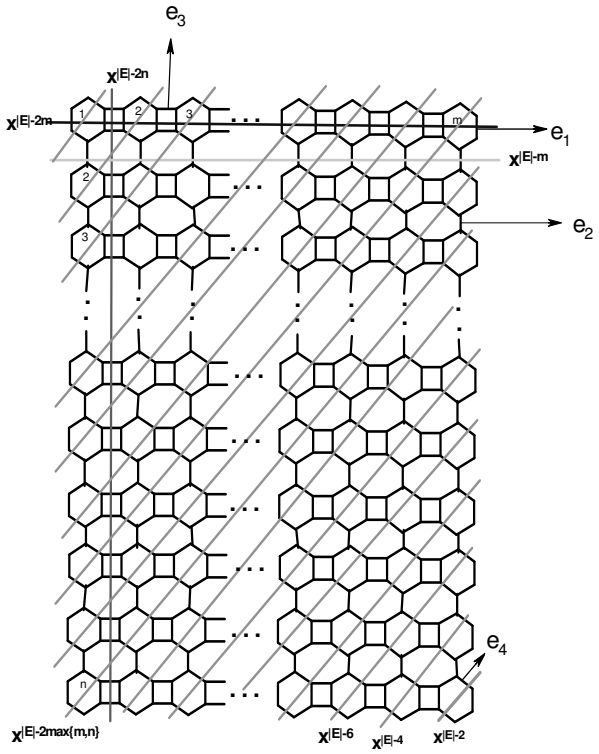

Fig. 1—The 2-dimensional graph K of the V-phenylenic nanotube.

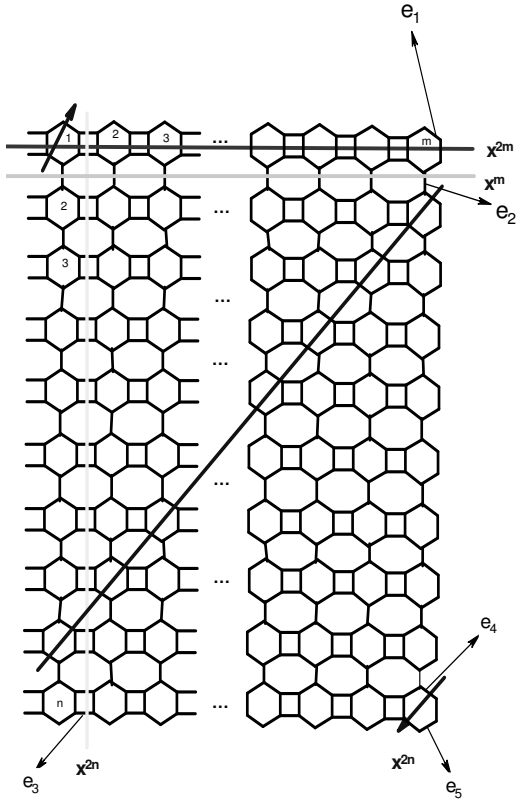

Fig. 2—The V-phenylenic nanotube G = VPHX[n,m].

above. The Sadhana polynomial of the 2-dimensional graph K (Fig. 1) is also computed. Following Diudea[20], we denote a V-Phenylenic nanotube by G = VPHX[n,m] and an V-Phenylenic nanotorus by H = VPHY[n,m] (Figs 2 and 3). It is easy to see that |V(G)| = |V(H)| = |V(K)| = 6mn, |E(G)| = 9mn – m, |E(H)| = 9mn and |E(K)| = 9mn – 2n – m. Yousefi-Azari *et al*.[26,27], computed the PI index of these nanotubes and nanotori.

We begin with the molecular graph of K (Fig. 1). One can see that there are four separate cases and that the number of qoc strips are different. Suppose e_1, e_2, e_3 and e_4 are representative edges for these cases. By definition of Sadhana polynomial and Table 1, one can see that

$$Sd(K,x) = 4\sum_{i=1}^{Max\{m,n\}-1} x^{|E(K)|-2i} + 2(|n-m|+1)x^{|E(K)|-2Min\{m,n\}} + nx^{|E|-2m} + (m-1)x^{|E|-2n} + (n-1)x^{|E|-m}$$

and so

$$Sd(K) = 36mn^2 - 3m^2 + 27m^2n - 8n^2 - 55mn + 10n + 5m.$$

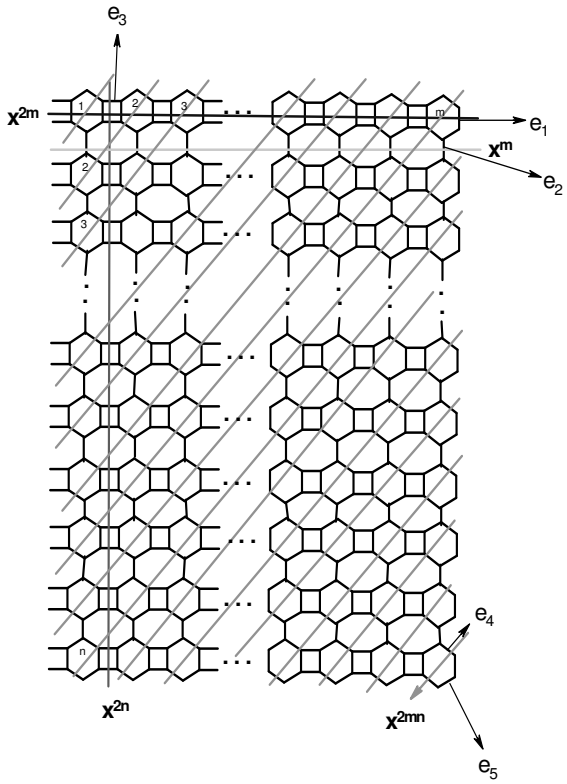

Fig. 3—The V-phenylenic nanotorus H = VPHY[n,m].

Table 1—The number of co-distant edges of e_i, $1 \le i \le 4$.

No.	Number of co-distant edges	Type of edges
n	2m	e_1
n-1	m	e_2
m-1	2n	e_3
4	2	e_4
4	4	
M	M	
4	$2\alpha-2$	
2(|m-n|+1)	2α	
	$\alpha=Max\{m,n\}$	

We now consider the molecular graph G (Fig. 2). Figure 2 shows that there are five different cases and the qoc strips are different. Suppose e_1, e_2, e_3, e_4 and e_5 are representatives of the different cases. Then our programs described in last section shows that $|C(e_1)| = 2m$, $|C(e_2)| = m$ and $|C(e_3)| = |C(e_4)| = |C(e_5)| = 2n$. On the other hand, there are n, n-1, m, m and m similar edges for each of edges e_1, e_2, e_3, e_4 and e_5, respectively. This implies that $Sd(G, x) = 3mx^{9mn-m-2n} + nx^{9mn-3m} + (n-1)x^{9mn-2m}$ and so $Sd(G) = 27m^2n + 18mn^2 - 3m^2 - 20mn + 2m$.

Figure 3 shows that there are five separate cases and the number of qoc strips are different. We denote these edges by e_1, e_2, e_3, e_4 and e_5. One can see that $|C(e_1)| = 2m$, $|C(e_2)| = m$ and $|C(e_3)| = 2n$, $|C(e_4)| = |C(e_5)| = 2mn$ (Fig. 3). On the other hand, there are n, n, m similar edges for each of edges e_1, e_2 and e_3, respectively. Therefore, $Sd(H, x) = 2x^{7mn} + nx^{9mn-2m} + mx^{9mn-2n} + nx^{9mn-m}$ and so $Sd(H) = 9m^2n + 18mn^2 + 9mn$.

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